

# **I Introduction**



# I. INTRODUCTION

## Developing Advanced Combustion Engine Technologies

On behalf of the Department of Energy's Office of FreedomCAR and Vehicle Technologies, we are pleased to introduce the Fiscal Year (FY) 2004 Annual Progress Report for the Advanced Combustion Engine R&D Sub-Program. The mission of the FreedomCAR and Vehicle Technologies Program is to develop more energy efficient and environmentally friendly highway transportation technologies that enable Americans to use less petroleum for their vehicles. The Advanced Combustion Engine R&D Sub-Program supports this mission by removing the critical technical barriers to commercialization of advanced internal combustion engines for light-, medium-, and heavy-duty highway vehicles that meet future Federal and state emissions regulations. The primary objective of the Advanced Combustion Engine R&D Sub-Program is to improve the brake thermal efficiency of internal combustion engines from

- 30 to 45 percent for light-duty applications by 2010
- 40 to 55 percent for heavy-duty applications by 2012

while meeting cost, durability, and emissions constraints. R&D activities include work on combustion technologies that increase efficiency and minimize in-cylinder formation of emissions, as well as aftertreatment technologies that further reduce exhaust emissions. Work is also being conducted on ways to reduce parasitic and heat transfer losses through the development and application of thermoelectrics and turbochargers that include electricity generating capability, and conversion of mechanically driven engine components to be driven via electric motors.

This introduction serves to outline the nature, current progress, and future directions of the Advanced Combustion Engine R&D Sub-Program. The research activities of this Sub-Program are planned in conjunction with the FreedomCAR Partnership and the 21st Century Truck Partnership and are carried out in collaboration with industry, national laboratories, and universities. Because of the importance of clean fuels in achieving low emissions, R&D activities are closely coordinated with the relevant activities of the Fuel Technologies Sub-Program, also within the Office of FreedomCAR and Vehicle Technologies.

Research is also being undertaken on hydrogen-fueled internal combustion engines to provide an interim hydrogen-based powertrain technology that promotes the longer-range FreedomCAR Partnership goal of transitioning to a hydrogen-fueled transportation system. Hydrogen engine technologies being developed have the potential to provide diesel-like engine efficiencies with near-zero emissions.

## Background

The compression ignition, direct injection (CIDI) engine, an advanced version of the commonly known diesel engine, is the most promising advanced combustion engine technology for achieving dramatic energy efficiency improvements in light- and heavy-duty vehicles. Light-duty hybrid vehicles using CIDI engines are projected to have energy efficiencies that are 80% higher than current gasoline vehicles, though the higher cost of CIDI engines relative to gasoline engines discourages use of this technology in light-duty applications right now. Implementation of the U.S. Environmental Protection Agency's (EPA's) Tier 2 regulations for light-duty vehicles, which took effect in 2004, is imposing another significant barrier to further penetration of CIDI engines in the U.S. This situation is unlike Europe, where diesel vehicles represent just over 50 percent of all new light-duty passenger car sales primarily because gasoline and diesel fuel are more expensive there but also because emission regulations are less stringent.

The CIDI engine is already the primary engine for heavy-duty vehicles because of its high efficiency and outstanding durability. However, the implementation of more stringent heavy-duty engine emission standards, which are to be phased in starting in 2007 (100% implementation in 2010), is predicted to cause a reduction in fuel efficiency due to the exhaust emission control devices needed to meet both the oxides of nitrogen ( $\text{NO}_x$ ) and particulate matter (PM) emissions regulations.



Cut-Away of DaimlerChrysler 3.2 L CIDI Engine that Achieves 30% Better Fuel Economy than its Gasoline Counterpart in Mercedes Light-Duty Vehicles

Given these challenges, the Advanced Combustion Engine Technologies Sub-Program is working toward achieving the following objectives:

- Advance fundamental combustion understanding to enable design of CIDI engines with inherently lower emissions. This will reduce the size and complexity of emission control devices and minimize any impact these devices have on vehicle fuel efficiency.
- Increase overall engine efficiency through fundamental improvements such as advanced combustion processes, reduction of parasitic losses, and recovery of waste heat.
- Improve the effectiveness, efficiency, and durability of CIDI engine emission control devices to enable these engines to achieve significant penetration in the light-duty market and maintain their application in heavy-duty vehicles.

## Technology Status

The technology for controlling PM emissions from CIDI engines is highly effective and is entering commercial markets in applications (mostly transit buses) where duty cycles and engine strategies create adequately high exhaust temperatures to ensure regeneration, and where ultra-low-sulfur fuel is available. The current light-duty diesel vehicles for sale in the U.S. (a few passenger car models and one small sport utility vehicle) rely on oxidation catalysts and/or advanced fuel injection and turbocharging to meet the standards for PM emissions. (Full-size pickups with diesel engines are not considered light-duty vehicles.) However, the lowest standard to which these vehicles are certified is Bin 9 (out of a total of 10), which limits their potential market penetration. Light-duty diesel vehicle manufacturers have indicated their desire to employ catalytic PM devices to further lower PM emissions once diesel fuel sulfur levels decrease to 15 ppm nationwide in June 2006. Cost and durability are likely to be the important characteristics for choosing which PM control technology to employ for a given application, though the type of  $\text{NO}_x$  control device used will also play a role in specifying a PM trap and where it will be placed. Regeneration strategies for light-duty vehicles need further development before these vehicles can be considered market-ready.

Technology for control of CIDI engine  $\text{NO}_x$  is not nearly as mature as the technology for control of PM. Competing technologies include adsorbers, selective catalytic reduction (SCR), lean- $\text{NO}_x$  catalysts (often called hydrocarbon-SCR), and non-thermal plasma (NTP)-assisted catalysis. Of these technologies, SCR using urea as a reductant is the current leader in terms of having the lowest fuel penalty and highest durability. In laboratory testing, Bin 3 emissions have been recorded, though full useful life is yet to be proven with new catalysts. Urea SCR faces the hurdle of requiring a urea distribution infrastructure to supply the vehicles. Heavy-duty vehicle manufacturers in Europe have committed to urea-SCR and are supporting urea distribution and dispensing infrastructure implementation and standards to assure urea quality. Serious discussions of the willingness of U.S. heavy-duty vehicle manufacturers to implement urea-SCR emission control are on-going. Urea-SCR is equally effective on light-duty CIDI vehicles, though development of urea distribution infrastructure is a more daunting prospect than for heavy-duty vehicles that primarily use truck stops for refueling. A system to refuel

light-duty CIDI vehicles with both diesel fuel and urea using one coaxial hose has been demonstrated and shows much promise. However, no proposal has been developed to assure that urea will be available at sufficient numbers of refueling facilities serving light-duty vehicles. Urea can also be stored onboard in solid pellet form, and enough can be stored to allow recharging at each oil change. This approach could make use of the current parts distribution system to recharge vehicles with urea.

Development of  $\text{NO}_x$  adsorbers has shown rapid improvement to the point that they appear to be able to achieve the Tier 2 Bin 5 light-duty vehicle emission levels when new using 4-ppm-sulfur fuel (which is lower than the average sulfur level expected for ultra-low sulfur fuel to be available after June 2006), though not for a full vehicle lifetime.  $\text{NO}_x$  adsorbers for heavy-duty vehicles are less well-developed based on the size of these units compared with engine displacement (being over twice as large as those required for light-duty vehicles). The durability of  $\text{NO}_x$  adsorbers is still in question since they are sensitive to even small amounts of sulfur in the fuel or engine lubricant (urea-SCR catalysts are less sensitive to sulfur). The other major concern about  $\text{NO}_x$  adsorbers is their effect on fuel consumption and cost.  $\text{NO}_x$  adsorbers use fuel to regenerate instead of urea, and current fuel "penalties" for regeneration are declining but still in the range of five to ten percent of total fuel flow. This is exacerbated by the need to periodically drive off accumulated sulfur by heating the adsorber to high temperatures, again by using fuel. These concerns must be addressed before  $\text{NO}_x$  adsorbers will be deemed to be commercially viable.



Prototype Diesel Fuel/Urea  
Co-Fueling Dispenser

Interest in lean- $\text{NO}_x$  catalysis (hydrocarbon-SCR) is making a bit of a come-back for use on both light- and heavy-duty CIDI vehicles. Currently, lean- $\text{NO}_x$  catalysts provide only 20-40 percent reduction in  $\text{NO}_x$ , but this may be sufficient when combined with measures to reduce engine-out  $\text{NO}_x$  such as exhaust gas recirculation (EGR), low-temperature combustion, or homogeneous charge compression ignition (HCCI). Lean- $\text{NO}_x$  catalysis may also be used as an interim step with heavy-duty engines as the 2007 standards are phased in. The advantages of lean- $\text{NO}_x$  catalysis include no core engine modifications, no fuel infrastructure requirements as for urea, some reduction of hydrocarbons and carbon monoxide, and being amenable to retrofit applications. Remaining drawbacks include catalyst activity and durability, the need for a broader operating temperature window, and lower selectivity leading to a higher fuel penalty.

Non-thermal plasma  $\text{NO}_x$  reduction catalysts have not achieved similar progress as competing technologies, and catalyst coking has been identified as a problem. Because of the lack of progress on NTP catalysis and its problems, the Advanced Combustion Technologies Sub-Program has decided to discontinue funding of this technology. Plasmas continue to be explored in reforming processes for generating diesel-fuel-based reductants for use with  $\text{NO}_x$  adsorbers.

An optimum solution to CIDI engine emissions would be to alter the combustion process in ways that produce emissions at levels that don't need ancillary devices for control, yet maintain or increase the engine efficiency. This is the concept behind new combustion regimes such as HCCI and other models of low-temperature combustion, which result in greatly reduced levels of  $\text{NO}_x$  and PM emissions (emissions of hydrocarbons and carbon monoxide still exist but are more easily controlled). Significant progress is being made in these types of combustion systems, and performance has been demonstrated over increasingly larger portions of the engine speed/load map. The major issues of this R&D include fuel mixing, combustion control, and extension of the operating range. Control of fuel injection and valve opening independent of piston movement appears to be necessary for HCCI engines to be viable. The optimum HCCI fuel has yet to be determined, though both diesel fuel and gasoline appear to be acceptable.

Complex and precise engine and emission controls will require sophisticated feedback systems employing new types of sensors.  $\text{NO}_x$  and PM sensors are in the early stages of development and require additional advances to be cost-effective and reliable, but are essential to control systems for these advanced engine/aftertreatment systems. Much progress has been made, but durability and cost remain the primary issues with these sensors.

Advanced fuel formulations and fuel quality are also crucial to achieving higher energy efficiencies and meeting emissions targets. The EPA rule mandating that sulfur content of highway diesel fuel be reduced to less than 15 ppm starting in 2006 will greatly benefit the effectiveness, durability, and life of emission control devices. The EPA has recently reported that based on pre-compliance reports, 95 percent of all the diesel fuel should be less than 15 ppm sulfur by June 2006.

## Future Directions

Internal combustion engines have a maximum theoretical fuel conversion efficiency that is similar to fuel cells; it approaches 100%. The primary limiting factor to achieving high fuel conversion efficiency is the high irreversibility in traditional premixed or diffusion flames. Multiple studies agree that combustion irreversibility losses consume more than 20% of the available fuel energy and are a direct result of flame front combustion. Examples of "new combustion regimes" that might lower the irreversibility losses include dilute combustion with low peak temperatures, higher expansion of combustion gases, and increased reactant temperature. The engine hardware changes needed to execute these advanced combustion regimes include variable fuel injection geometries, methods to produce very high manifold pressures, compound compression and expansion cycles, and improved sensors and control methods.

The other areas where there is large potential for improvements in internal combustion engine efficiency are losses from the exhaust gases and heat transfer losses. Potential ways that these losses might be reduced include compound compression and expansion cycles achieved by valve timing, use of turbine expanders, application of thermoelectric generators, and lean-burn and stratified-charge engines.

Fuels can also play an important role in reducing combustion irreversibility losses. Preliminary analyses show that combustion irreversibility losses per mole of fuel are considerably less for hydrogen than for hydrocarbon fuels. This is consistent with the understanding that combustion irreversibility losses are reduced when combustion is occurring nearer equilibrium (high temperature), since hydrogen has the highest adiabatic flame temperature of the fuels studied to date. This bodes well for the development of highly efficient hydrogen-fueled internal combustion engines.

## Goals and Challenges

Quantitative targets have been developed for advanced engines in three major applications: passenger cars, light trucks, and heavy trucks. Light trucks here refer to pickup trucks, vans, and sport utility vehicles that are emissions-certified to the same standards as passenger cars, or generally "light-duty vehicles." Fuel efficiency improvement is the overarching focus of this Sub-Program, but resolving the interdependent emissions challenges is a critical first step. (Penetration of even current technology CIDI engines into the light-duty truck market would reduce fuel use by 30-40% per gasoline vehicle replaced.) The major challenges facing CIDI emission control systems across all three platforms are similar: durability, cost, and fuel penalty (or in the case of urea-SCR, urea infrastructure development). Full-life durability has yet to be demonstrated for either light- or heavy-duty systems. Nor have these systems demonstrated their ability to "bounce back" following exposure to fuel sulfur levels higher than 15 ppm, which could occur periodically due to cross-contamination of fuels and outright fuel substitution mistakes. With significant progress made toward emission controls, attention will be turned more toward engine efficiency improvements by improving combustion and systematically attacking losses such as friction, exhaust energy, heat transfer, and parasitic losses.

The targets for passenger cars, derived primarily by the FreedomCAR Partnership, are shown in Table 1. Achieving emissions compliance for CIDI engines in light-duty vehicles will provide a "quantum leap" (~30%) fuel efficiency improvement over port-fuel-injected spark ignition engines. In the longer term, further advancement of engine efficiency along with reducing the emission control penalty will gain another 15-18% beyond today's technology.

**Table 1.** Technical Targets for Combustion and Emission Control Activity

Characteristics	Units	Fiscal Year		
		2004	2007	2010
FreedomCAR Goals				
ICE Powertrain				
Peak Brake Thermal Efficiency (CIDI/H <sub>2</sub> -ICE) (H <sub>2</sub> -ICE)	%			45/45 45 (2015)
Cost (CIDI/H <sub>2</sub> -ICE) (H <sub>2</sub> -ICE)	\$/kW			30/45 30(2015)
Reference Peak Brake Thermal Efficiency <sup>a</sup>	%	30	32	34
Target Peak Brake Thermal Efficiency/Part-Load Brake Thermal Eff. (2 bar BMEP <sup>b</sup> @1500 rpm)	%	43/29	45/32	46/35
Powertrain cost <sup>c,d</sup>	\$/kW	30	30	30
Emissions <sup>e</sup>	g/mile	Tier 2, Bin 5	Tier 2, Bin 5	Tier 2, Bin 5
Durability <sup>e</sup>	Hrs.	5,000	5,000	5,000
Fuel efficiency penalty due to emission control devices <sup>f</sup>	%	<5	<3	<1

<sup>a</sup>Current production, EPA-compliant engine

<sup>b</sup>Brake mean effective pressure

<sup>c</sup>High-volume production: 500,000 units per year

<sup>d</sup>Constant out-year cost targets reflect the objective of maintaining powertrain (engine, transmission, and emission control system) system cost while increasing complexity.

<sup>e</sup>Projected full-useful-life emissions for a passenger car/light truck using advanced petroleum-based fuels as measured over the Federal Test Procedure as used for certification in those years.

<sup>f</sup>Energy used in the form of reductants derived from the fuel, electricity for heating and operation of the devices, and other factors such as increased exhaust back-pressure which reduces engine efficiency.

The light truck diesel engine R&D activity will not be continued past this year. All the 2004 targets listed in Table 2 have been demonstrated to be achievable with the exception of emission controls that have full-useful-life durability. The availability of commercial products having these characteristics depends on manufacturers doing the necessary product engineering and durability testing.

**Table 2.** Technical Targets for Light Truck Diesel Engine R&D

Characteristics	Units	2004
Engine power	hp	225-325
Fuel economy increase over equivalent gasoline vehicles	%	>50
Engine cost (compared to equivalent gasoline engine)	%	<120
Engine weight (compared to equivalent gasoline engine)	%	<110
NVH <sup>a</sup> (compared to equivalent gasoline engine)	db difference	<1
NO <sub>x</sub> emissions <sup>b</sup>	g/mile	<0.07
PM emissions <sup>b</sup>	g/mile	0.01
Durability <sup>c</sup> (on lab dynamometer, computer simulated vehicle miles)	miles (equivalent)	>100,000

<sup>a</sup>Noise, vibration, and harshness<sup>b</sup>Projected full-useful-life emissions for a SUV (using advanced petroleum-based fuels with 15 ppm sulfur) as measured over the Federal Test Procedure as used for certification in those years.<sup>c</sup>Projected full-useful-life durability, as measured over the Federal Test Procedure as used for certification.

Heavy truck engine R&D activities are focused on increasing heavy-duty diesel engine efficiency significantly above current levels as well as addressing efficiency penalties resulting from emission control technologies required to meet the increasingly stringent emissions standards. As seen in Table 3, heavy-duty truck engines will need to simultaneously increase thermal efficiency significantly while lowering emissions and doubling durability, all by the end of 2005. To date, all the 2005 targets have been achieved except for emissions systems durability. By 2007, efficiency will need to be increased further while NO<sub>x</sub> emissions are reduced and durability doubled over that required to meet the 2005 target. Achieving these technical targets will require sustained R&D activities along several fronts.

**Table 3.** Technical Targets for Heavy Truck Diesel Engine R&D

Characteristics	Fiscal Year			
	2002 Status	2005	2007	2012
Engine thermal efficiency, %	>40	>45	>50	>55
NO <sub>x</sub> emissions, <sup>1</sup> g/bhp-hr	<2.0	<1.2	<0.20	<0.20
PM emissions <sup>1</sup> , g/bhp-hr	<0.1	<0.01	<0.01	<0.01
Stage of Development	commercial	prototype	prototype	prototype
Durability, miles (equivalent)	>100,000	>200,000	>400,000	

<sup>1</sup>Using 15-ppm-sulfur diesel fuel

Recovery of energy from the engine exhaust represents a potential for 10 percent or more improvement in the overall engine thermal efficiency. More efficient turbochargers using variable geometry and electric assist are one approach. Turbocompounding and direct thermal-to-electric conversion could also improve the overall thermal efficiency. Semiconductor thermoelectric devices are currently 6 to 8 percent efficient, but recent developments in quantum well thermoelectrics suggest an improvement to over 20 percent is possible. The technical targets for the waste heat recovery R&D activities are listed in Table 4. Significant progress will be needed to meet the 2005 and 2008 targets. Newly awarded projects are focused on achieving this progress.



**Table 4.** Technical Targets for Combustion and Emission Control Activity

Characteristics	Units	Fiscal Year		
		2003 Status	2005	2008
Electrical turbocompound system				
Light-Duty Vehicles				
Power	kW	<2	>5	>10
Projected component life	Hrs.	<10	>2,000	>5,000
Class 7-8 trucks				
Fuel economy improvement	%	<1	>5	>10
Power	kW	<10	>20	>30
Projected component Life	Hrs.	<10	>5,000	>10,000
Thermoelectric Devices				
Efficiency bulk semiconductor quantum well	%	6-8	-- >10	-- >15
Projected cost @ 250,000 production volume	\$/kW	--	500	180

## Project Highlights

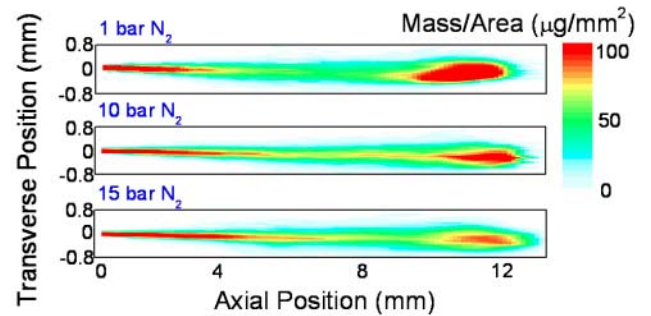
The following projects highlight progress made in the Advanced Combustion Engine R&D Sub-Program during FY 2004.

## Advanced Combustion and Emission Control Research for High-Efficiency Engines

### A. Combustion and Related In-Cylinder Processes

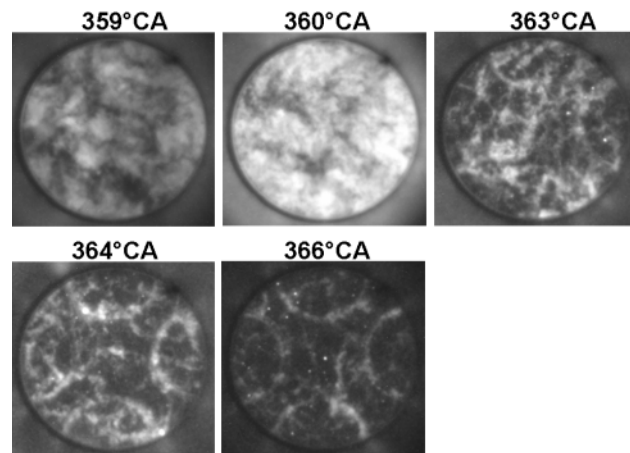
The objective of these projects is to identify how to achieve more efficient combustion with reduced emissions from advanced technology engines.

- Argonne National Laboratory (ANL) expanded their x-ray fuel spray measurement technique to inject in atmospheres at pressures of 15 and 20 bar. They also demonstrated for the first time that the x-ray technique can be useful for resolving subtle differences in the sprays based on the internal structure of the nozzle.
- Sandia National Laboratories (SNL) experimentally evaluated a late-injection, low-temperature diesel combustion regime for a wide variety of system parameters, including injection pressure, swirl ratio, O<sub>2</sub> concentration (exhaust gas recirculation rate), start of injection, and intake temperature. The optimum swirl level and rate-limiting factors at various stages of the combustion process were identified.
- SNL demonstrated that diesel combustion is soot-free for an ambient gas oxygen concentration of 8% and typical diesel ambient gas temperature (1000 K). They also found that combustion efficiency remains high for mixing-controlled diesel combustion with flame temperatures as low as 1500-1600 K for conditions where the ambient gas temperature is greater than 1000 K.

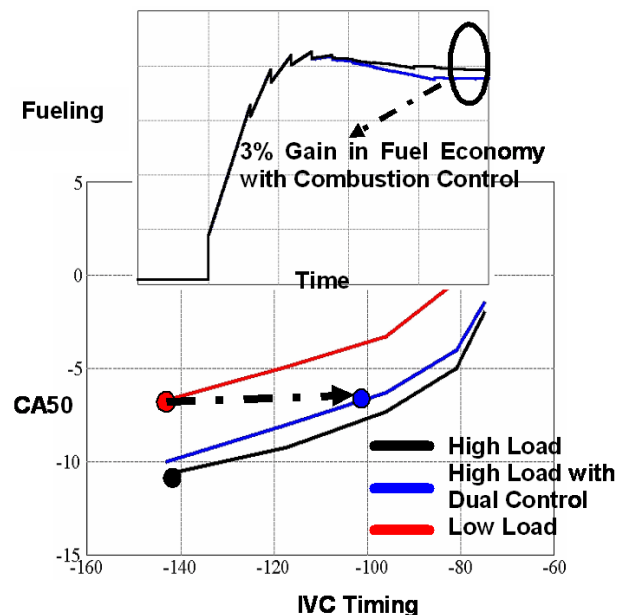


Differences in Fuel Spray Penetration with Pressure Revealed by X-Rays

- Using only high EGR and specific engine operating parameters, Oak Ridge National Laboratory (ORNL) demonstrated rapid transition between conventional combustion and a high-efficiency clean combustion mode in a production light-duty CIDI diesel engine with 90% reduction in engine-out NO<sub>x</sub> and a 50% reduction in PM emissions under road-load type conditions (20% load, 1500 rpm) without excessive hydrocarbon (HC) emissions.
- Lawrence Livermore National Laboratory (LLNL) extended their combustion multi-zone analysis methodology to make it applicable to analysis of premixed charge compression ignition (PCCI), a generalization of HCCI combustion where the fuel and air mixture may be partially stratified at the moment of ignition.
- SNL conducted an investigation of the lowest temperature for complete combustion of hydrocarbon fuels over a wide range of conditions. They showed that the peak temperature must exceed 1500 K at 1200 rpm, regardless of fuel type or combustion timing.
- SNL identified several tracers that improve fuel tracking by better matching the volatility of reference fuels.
- The University of Wisconsin identified diesel HCCI combustion regimes in a Caterpillar 3401 engine using both low-pressure and high-pressure multiple injection strategies. They also developed models that minimize fuel deposition on the walls and provide start-of-combustion control via variable valve timing and variable geometry sprays.
- The University of Michigan experimentally demonstrated potential HCCI engine control methods using valve control and thermal effects and identified that valve control has characteristic response times of 10's of cycles while thermal effects are on the order of 100's of cycles.
- Caterpillar developed a novel HCCI engine system that successfully achieves the proper air-fuel mixture using conventional diesel fuel and achieved 2100+ kPa brake mean effective pressure (BMEP) while meeting future emissions standards. This is the highest known power density in the world achieved using any form of HCCI.
- ORNL demonstrated that HCCI combustion in a gasoline engine could improve fuel economy by an average of 12% while reducing NO<sub>x</sub> emissions by 95% compared to conventional combustion.
- ORNL (as part of their CRADA with Detroit Diesel Corporation [DDC]) performed extensive experiments under low and medium load conditions to characterize the effects of EGR rate, rail pressure,



Images of HCCI Combustion Using Laser Imaging



Estimate of Fuel Consumption Reduction with Application of HCCI Combustion

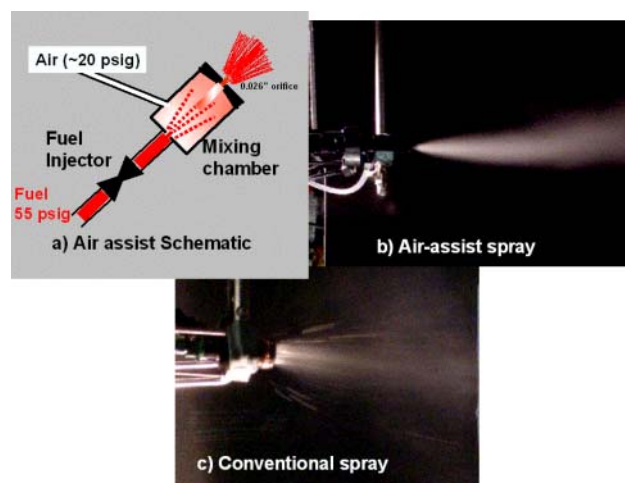
and injection timing on achieving high-efficiency clean combustion operation of a current DDC diesel engine.

- Los Alamos National Laboratory (LANL) modified all subroutines of KIVA-3V to accommodate unstructured grids. A beta version of KIVA-4 has been distributed to the industry Memorandum of Understanding participants.
- LLNL developed models for chemical kinetics of combustion of two major fuel components, toluene and methyl cyclohexane, and for an oxygenated diesel fuel additive, dimethyl carbonate.

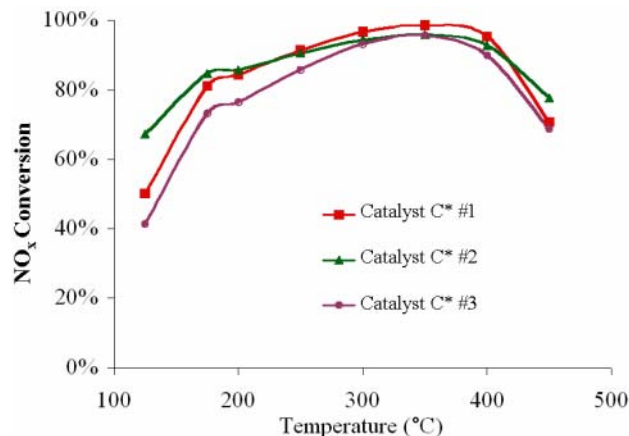
## B. Energy-Efficient Emission Controls

The following project highlights summarize the advancements made in emission control technologies to both reduce emissions and reduce the energy needed for their operation.

- Pacific Northwest National Laboratory (PNNL) identified cryptomelane, an octahedral molecular sieve based on manganese cations, as a stoichiometric  $\text{SO}_2$  absorber having total capacity of approximately 70 wt.% and a breakthrough capacity of 60 wt.% at 325°C. The capacity of the material is virtually unaffected with realistic feeds under cyclic lean-rich conditions.
- ORNL (as part of a CRADA with International Truck and Engine) developed a strategy for regenerating  $\text{NO}_x$  adsorbers at rated load (600°C) to meet the NTE (not-to-exceed) emission standards and achieved 70%  $\text{NO}_x$  reduction at rated power, with acceptable CO and HC emissions and very low fuel penalty (<2.5%).
- ANL demonstrated that paraffins are ineffective as reductants for their deNO<sub>x</sub> catalyst and that aromatics (toluene and xylenes) are highly effective while selectivity to  $\text{N}_2$  still remains near the 100% mark.
- ORNL developed a draft bench characterization protocol for lean  $\text{NO}_x$  trap (LNT) materials in conjunction with supplier representatives and the LNT Focus Group that is intended to provide the basis of standard kinetic 'maps' (i.e., data templates) for communicating critical simulation properties. ORNL presented the protocol at the 7th CLEERS workshop and posted it on the web.
- Ford achieved low-mileage Tier 2 Bin 5 standards using a fresh catalyst system of oxidation catalysts, urea-SCR and a catalyzed diesel particulate filter (CDPF) in a mid-sized diesel prototype engine designed for a light-duty truck. Engine-out  $\text{NO}_x$  was lowered by 40% through the use of a cooled, low-pressure EGR system.



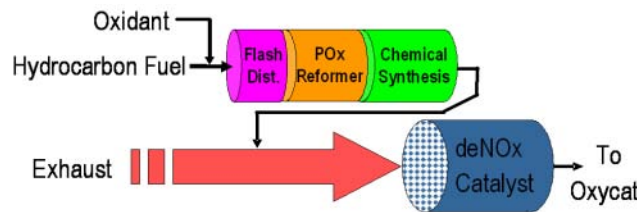
Air-Assisted Fuel Injector for Regenerating  $\text{NO}_x$  Adsorbers



New Catalysts Are Being Discovered that Have High  $\text{NO}_x$  Conversion Efficiency

- LANL achieved milestone  $\text{NO}_x$  conversion efficiency of >95% between 160 and 400°C at a gas hourly space velocity (GHSV) of 30,000  $\text{h}^{-1}$  and  $\text{NO}:\text{NO}_2 = 4:1$  using a 'hybrid' dual-bed base metal zeolite catalyst system supported on a monolith.

- PNNL invented a new catalyst material (disclosure filed) that shows excellent activity for hydrocarbon SCR of simulated diesel exhaust without the need for a plasma device.
- ORNL developed a testing procedure for measuring thermal deactivation that simulates 400,000 miles of operation in a 15-hour test. They also demonstrated poisoning effects of sulfur in model LNT catalysts using a test procedure that simulates 126,000 miles of operation.
- Noxtech demonstrated over 94% reduction of  $\text{NO}_x$  from the exhaust of a high-speed diesel engine under conditions of  $30,000 \text{ hr}^{-1}$  space velocity while using 50 ppm sulfur fuel.
- Using reductants developed from fuel oxygenates, PNNL demonstrated 70%  $\text{NO}_x$  reduction activity, which is significantly greater than conventional lean- $\text{NO}_x$  performance of 40%.
- General Motors tested over 3000 materials for  $\text{NO}_x$  reduction potential and identified multiple hydrocarbon SCR materials that enable  $\text{NO}_x$  conversion in excess of 80%.



Schematic of a Reductant Preparation System for Lean- $\text{NO}_x$  Catalysts

### C. Critical Enabling Technologies

- Sensors, new instrumentation, and advanced catalyst designs are enabling technologies for achieving more efficient engines with very low emissions. The following highlights show the progress made during FY 2004.
- Caterpillar produced prototype metal substrates for catalytic converters that have similar long-term cyclic oxidation resistance as current ceramic-based substrates. Metal substrates are less costly and allow smaller designs with less substrate weight and precious metal content.
- Delphi continued development of a  $\text{NO}_x$  sensor by improving sinterability of the sensing element, developing a key electrode material, eliminating cross contamination of electrode materials through improved design, and implementing an advanced interconnection design.
- CeramPhysics successfully manufactured capacitor-type combined  $\text{NO}_x$  and  $\text{O}_2$  sensor bodies with two types of porous Rh-based electrodes.
- PNNL developed a ceramic oxygen pumping electrode for an  $\text{NO}_x$  sensor that is compatible with high sensor processing temperatures, shows very high activity for oxygen pumping, is insensitive to  $\text{NO}_x$ , and should be less costly than noble metal electrodes.
- ANL developed a portable PM emissions measurement system and successfully demonstrated it onboard an operating diesel vehicle.
- SNL developed a laser-induced incandescence PM measuring instrument and tested it at several industry laboratories as well as at ORNL, demonstrating high accuracy, fast response, and high reliability without the



Prototype  $\text{NO}_x$  Sensors



Test of Portable Laser-Based PM Measurement Instrument



need for operator oversight. Artium Technologies Inc., in Sunnyvale, California, is commercializing this instrument, and the first commercial sales occurred in the spring of 2004.

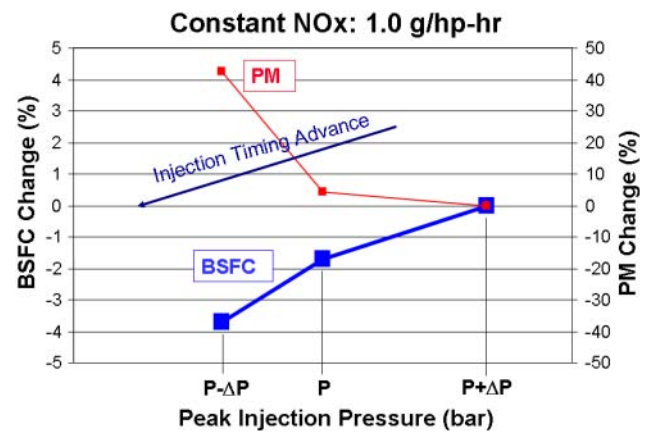
- Honeywell established the feasibility of monitoring particulates directly in the exhaust manifold without pretreatment or dilution and without sensor fouling due to accumulation of particulate matter. Concept prototype PM sensors have been fabricated for testing.

## Advanced Engine Designs for Improved Efficiency

With the advent of stringent emission standards, it is necessary to design engines as systems to achieve both high efficiency and low emissions. The following project highlights describe the progress made for both light- and heavy-duty engines during FY 2004.

### A. Heavy-Duty

- Cummins achieved and demonstrated 45% brake thermal efficiency while meeting 2007 emissions goals. They also demonstrated an advanced recirculated exhaust gas cooling system and evaluated different forms of homogeneous charge compression ignition combustion.
- Caterpillar built a demonstrator truck with 2007 emissions technology that has provided key insight into system integration challenges and real driving cycle performance. They also demonstrated full-load and full-power HCCI operation on a single-cylinder test engine while achieving 2010 emissions levels and demonstrated the potential of NO<sub>x</sub> aftertreatment to achieve 2010 emissions levels on a multiple-cylinder engine.
- DDC achieved 43% brake thermal efficiency in a multi-cylinder engine configuration while demonstrating engine-out NO<sub>x</sub> and particulate matter (PM) emissions of 1.1 g/hp-hr and 0.1 g/hp-hr, respectively, over the hot cycle Federal Test Procedure (FTP). They also subsequently demonstrated tailpipe-out NO<sub>x</sub> and PM emissions of ~1.0 g/hp-hr and <0.01 g/hp-hr, respectively, with integration of a diesel particulate filter.



Trade-Off of PM Emissions and Efficiency at Constant Low NO<sub>x</sub> Emissions

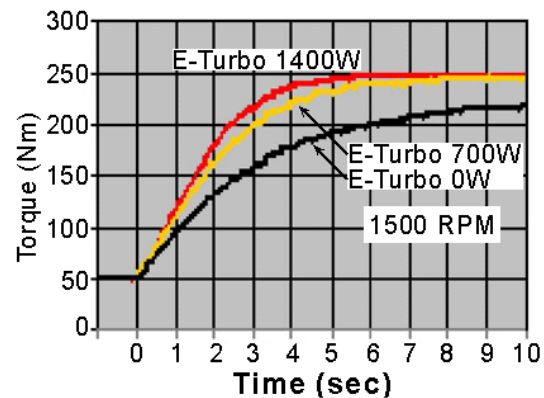
### B. Light-Duty

- Cummins demonstrated power density of 48 HP/liter on a 4.2-liter V6, and Tier 2 Bin 5 emissions capability through emissions testing at sea level and at altitude with 150,000 mile thermally aged catalyst.
- DDC demonstrated Tier 2 Bin 3 emissions over the FTP75 cycle for a light-duty diesel truck (LDT) equipped with a diesel particulate filter and urea-based selective catalytic reduction (DPF + SCR) system. This aggressive reduction in emissions was obtained without ammonia slip and with a 41% fuel economy improvement compared to the equivalent gasoline engine equipped vehicle. DDC also demonstrated Tier 2 emissions compliance over the US06 cycle.
- Modeling of the Envera variable compression ratio system projected part-load efficiency to be higher than that of the DaimlerChrysler A170 common-rail turbo-CDI current production engine (representative of current design CIDI engines).

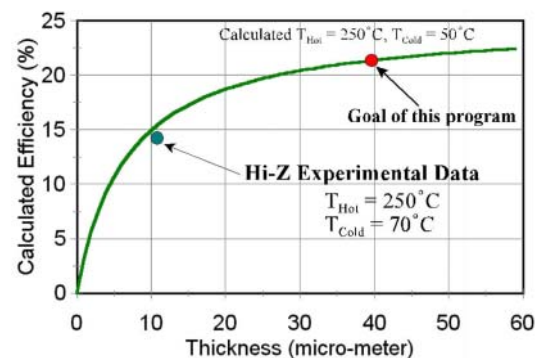
## Waste Heat Recovery

Two technologies are being pursued to capture waste heat from advanced combustion engines: electricity generation from turbochargers and thermoelectrics. Following are highlights of the development of these technologies during FY 2004.

- Honeywell developed an enhanced version of their e-Turbo™ system. The electricity generated by the turbocharger was shown to lower brake specific fuel consumption at steady-state engine operation by up to 6%. Using the e-Turbo™ system in reverse (i.e., as power assist to the turbocharger) allows low-speed torque to be increased, resulting in potential to reduce engine size by 10-30% with the same vehicle performance. Such engine downsizing could reduce fuel use by 6-17%.
- Hi-Z Technology, Inc. has achieved >530,000 equivalent miles in road tests of their 1-kW diesel truck thermoelectric generator. Post durability test inspection found that the internal resistance increased from 0.6 to 0.75 Ohms. This increase could be partially attributable to electrical contact corrosion. Hi-Z assembled and tested two different single-couple modules, and the conversion efficiency from both tests was in excess of 14% at a temperature differential of 200°C.
- PNNL scaled up the deposition process for multilayer thermoelectric substrates to 0.5 m<sup>2</sup> in area and demonstrated prototype batch deposition. They also established measurements of thermoelectric properties of thin films at temperatures up to 800°C.



Improved Engine Response from Use of an Electrically-Assisted Turbocharger

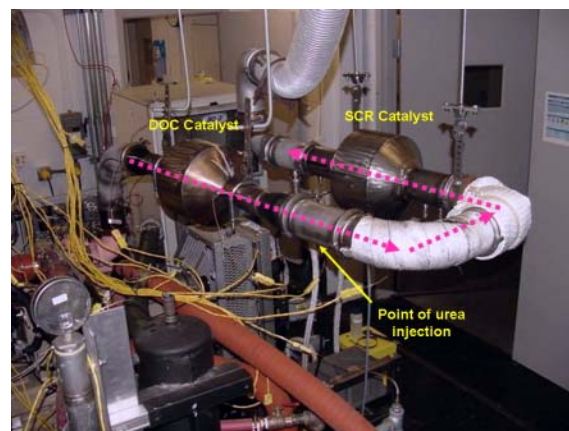


Advancements in Thermoelectric Generator Efficiency

## Off-Highway Vehicle Engine R&D

Off-highway vehicles are coming under more stringent emission controls similar to those for highway vehicles. However, their typical duty cycles place unique demands on emission control systems. Following are highlights of off-highway vehicle efficiency improvement and emission control development during FY 2004.

- Cummins designed and optimized engine combustion to achieve compliance with Tier 3 emission levels without the use of EGR and with only a slight degradation in fuel consumption for certain engine models. Work is proceeding on achievement of Tier 4 emission standards.
- John Deere used cooled low-pressure loop EGR and a continuously regenerating diesel particle filter (CR-DPF) to meet Tier 3 emissions with slightly improved fuel consumption.



Test Set-Up of Urea-SCR System for Off-Road Engines

- The Electromotive Division of GM completed engine test results showing that their new fuel injection system has the potential to meet locomotive Tier 2 emissions goals with favorable NO<sub>x</sub>-BSFC-PM (oxides of nitrogen - brake specific fuel consumption - particulate matter) trade-off characteristics.
- General Electric developed a computational fluid dynamics model to guide development of an advanced fuel injection system. They also designed, built, and tested an electrically assisted turbocharger and evaluated candidate abrasion-resistant seal materials identified for the turbocharger compressor and turbine shrouds.
- ORNL, in a CRADA with John Deere, demonstrated that a urea-SCR system could meet Tier 4 emissions for off-highway diesel engines. Improved fuel efficiency was also demonstrated through the application of an advanced fuel injection system.

## **Future Directions**

### **Advanced Combustion and Emission Control Research for High Efficiency Engines**

#### A. Combustion and Related In-Cylinder Processes

- ANL plans to increase the pressure capability of their x-ray fuel spray technique and make upgrades to enable the use of production fuel injector nozzles. They also plan to make improvements in the system including faster data acquisition, processing, and analysis; improved x-ray detector systems; increased x-ray intensity; and greater automation.
- SNL will evaluate alternative low-temperature combustion systems and identify the rate-limiting factors that prevent their application over a wider speed/load range.
- SNL will investigate how very high EGR affects diesel soot formation by performing quantitative measurements for ambient oxygen concentrations ranging from 21% to 10%.
- ORNL plans to investigate techniques for entering and exiting high-efficiency and low-emission combustion modes for CIDI diesel engines and consider potential diagnostic tools for feedback control when transitioning between these modes.
- LLNL will develop combustion analysis tools to accurately predict combustion and emissions under PCCI combustion.
- SNL plans to combine multi-zone Senkin modeling with experimental data to investigate how thermal stratification affects HCCI heat release rates with normal and retarded timing, and to determine the potential for extending the high-load limit with thermal stratification.
- SNL will characterize the charge-preparation process for HCCI engines using alternative injectors and injection strategies, including liquid injection, wall wetting, and fuel-air mixing.
- The University of Wisconsin plans to assess the use of multiple injections for diesel HCCI combustion control.
- The University of Michigan will continue engine control experiments to expand and refine current studies of mode transitions and thermal transients necessary for successful HCCI implementation.
- Caterpillar will focus on identifying and developing a cost-effective method of manufacturing the HCCI engine system they have developed.
- ORNL plans to continue to evaluate and quantify the use of spark augmentation for gasoline HCCI engine control and transition to HCCI combustion.
- ORNL (as part of their CRADA with DDC) will explore the potential of achieving HCCI-like operation and further expanding the range of high-efficiency clean combustion operation of a heavy-duty multi-cylinder diesel engine.

- LANL plans to assemble a KIVA-4 manual, develop a KIVA-3V mesh converter which will convert KIVA-3V meshes to KIVA-4 format, continue validation of KIVA-4 by adding to the existing test suite of engine problems, and develop and begin implementing a grid-generation strategy for KIVA-4 that incorporates commercial grid-generation packages.
- LLNL will extend model capabilities to additional classes of fuel components and continue development of increasingly complex surrogate fuel mixtures.

#### B. Energy-Efficient Emission Controls

- PNNL will continue studies with metal-modified cryptomelane to further increase SO<sub>2</sub> uptake capacity at 200°C and below, and develop and characterize alternate SO<sub>2</sub> adsorbents having moderate SO<sub>2</sub> capacity that can be regenerated on the vehicle during the rich cycle.
- ORNL (as part of a CRADA with International Truck and Engine) plans to measure the sulfur compounds that are released from desulfurizing an NO<sub>x</sub> adsorber catalyst and re-examine NTE and lower temperature conditions with in-pipe injection of pure compounds.
- ANL will test several optimized deNO<sub>x</sub> catalysts on an engine in a test cell using a slip stream of the diesel feed as the reductant. Optimization will include maximizing space velocity while minimizing the catalyst volume.
- ORNL will demonstrate the draft LNT characterization protocol on the ORNL bench-flow reactor and identify needed revisions and technical issues.
- Ford plans to conduct durability testing of their light-duty diesel truck emission control system and continue laboratory testing/development of ammonia sensing technologies to determine their value in a urea-SCR diesel aftertreatment system.
- ORNL will elucidate sulfur-based deactivation mechanisms and chemistry by determining the chemical form of sulfur-based species, identifying the desulfation temperatures for each sulfur species, and evaluating intermediate species formations to determine their chemistry.
- Noxtech plans to use the data generated from the 60-kW engine test to design, build and evaluate a system capable of reducing the NO<sub>x</sub> from a 250-kW high-speed diesel engine by over 90%.
- PNNL will investigate additional oxygenates as reductants for lean-NO<sub>x</sub> traps and alternate methods of reductant production.
- General Motors plans to continue the discovery of materials with good low-temperature NO<sub>x</sub> conversion properties to assist with cold-start emission reduction, and to scale up the promising materials for engine testing.

#### C. Critical Enabling Technologies

- Caterpillar will complete testing of full-scale current design metal substrate catalyst prototypes with new materials, including hot shake tests; complete modeling of the new design to determine optimum geometry to maximize activity while minimizing backpressure; and produce a full-scale prototype of new design substrate with optimized geometry and new material.
- Delphi plans to evaluate their NO<sub>x</sub> sensor subsystem in bench testing and on a running engine.
- CeramPhysics will incorporate NO<sub>x</sub> and O<sub>2</sub> sensor bodies into fully assembled NO<sub>x</sub> sensors and complete testing of them at an outside laboratory.
- PNNL plans to determine how their NO<sub>x</sub> sensor operation is affected by the presence of ammonia in exhaust gases, and investigate pulsed detection methods as a means of enhancing sensor sensitivity and accuracy.
- ANL will complete tests evaluating the sensitivity of their portable PM measuring instrument to the volatile organic fraction of PM, and explore the possibility to incorporate the capability to measure particle aggregate size and number density.



- SNL plans to improve the capabilities of their laser-induced incandescence PM measuring instrument and continue the collaboration with Artium Technologies toward commercialization of instrumentation for PM measurements.
- Honeywell will demonstrate prototype PM sensors and electronics in several end-user facilities.

## **Advanced Engine Designs for Improved Efficiency**

### **A. Heavy-Duty**

- Cummins will perform engine system modeling to predict engine, aftertreatment, and heat recovery system performance and perform test cell testing to verify the models developed and system performance.
- Caterpillar plans to focus on developing supporting engine systems to facilitate full-load HCCI on a multiple-cylinder engine and on developing methods and techniques to overcome NO<sub>x</sub> aftertreatment durability problems. Fuel efficiency, cost and manufacturability will also be areas of focus for these technologies.
- DDC will evaluate advanced fuel injection equipment, including hybrid systems, for the potential to enable combustion characteristics that will lead to over 45% thermal efficiency while meeting 2010 regulated emissions.

### **B. Light-Duty**

- A variable compression ratio (VCR) variant of the DaimlerChrysler 1.7L 4-cylinder common-rail turbo-diesel will be used to investigate compression direct injection (CDI) emissions, fuel economy, and advanced combustion benefits that can be attained with VCR.
- The ability to attain 25 percent improvement in spark ignition engine fuel economy with HCCI combustion using VCR and adjustable valve settings for controlled combustion from idle to high load levels will be demonstrated through hardware testing and computer modeling.
- The ability to attain 30 percent improvement in fuel economy with VCR, supercharging, and engine downsizing at significantly lower production cost than hybrid electric vehicle (HEV) technology (dollars per percent increase in fuel economy) while meeting federal and state emission standards will be demonstrated through hardware testing and computer modeling.

## **Waste Heat Recovery**

- DOE will award new cooperative agreements to develop thermoelectric devices and turbo-compounding units to convert waste heat to electricity.
- Honeywell will develop and demonstrate a 3rd-generation improved prototype e-Turbo design.
- Caterpillar will focus on engine testing of their complete electric turbocompound system.
- Hi-Z plans to accelerate quantum well development with the installation and startup of the 34-inch ID fabrication machine and test 2½-watt and larger modules.
- PNNL will develop Si/Si<sub>0.8</sub>Ge<sub>0.2</sub> and B<sub>4</sub>C/B<sub>9</sub>C multilayer structures on non-crystalline substrates and conduct thermoelectric performance measurements up to 800°C.

## **Off-Highway Vehicle Emission Control R&D**

- DOE will award new cooperative agreements to improve the efficiency of off-highway engines while meeting future emission standards.
- General Electric will continue to develop advanced fuel injection system and combustion technologies for locomotive application.
- Cummins will develop technologies including engine and aftertreatment solutions to meet the Tier 4 emissions levels at Tier 3 fuel consumption levels.

- John Deere will switch to a 6.8-liter, more advanced diesel engine and reduce the NO<sub>x</sub> from 4 to 2 g/kWh to meet the interim Tier 4 (2011) off-highway emission standards. The exhaust aftertreatment will be upgraded to the latest technology for better performance.
- The Electromotive Division of General Motors plans to complete the remaining single-cylinder engine tests and spray imaging experiments at Argonne National Laboratory, and computational fluid dynamics studies on cavitation at Wayne State University.
- ORNL (John Deere CRADA) plans to explore the potential for other NO<sub>x</sub> reduction strategies to meet final Tier 4 NO<sub>x</sub> and PM emissions, and conduct further urea-SCR studies to optimize NO<sub>x</sub> conversion with selected injection control strategies for lower BSFC.

## Honors and Special Recognitions

- Chris Powell, et. al, of ANL were awarded "Best Paper" for "Comparison of X-Ray Based Fuel Spray Measurements with Computer Simulation Using the CAB Model" presented at the ASME/CIMAC Congress 2004, Kyoto, Japan, June 2004.
- Chris Powell of ANL received an SAE "Excellence in Oral Presentation" award for presentation of a paper on spray research using x-ray radiography.
- Paul Miles received an SAE "Excellence in Oral Presentation" award for presentation of his paper on low-temperature automotive diesel combustion, SAE Paper 2004-01-1678, in March 2004.
- Paul Miles received a Sandia National Laboratories Employee Recognition Award for Individual Technical Excellence, June 2004, for his work on low-temperature automotive diesel combustion.
- Paul Miles and Richard Steeper of SNL were selected as Co-Vice-Chairs of Combustion for SAE's Fuels and Lubricants Activity.
- The Lawrence Livermore National Laboratory (LLNL) HCCI work was featured in the April 2004 issue of LLNL's "Science and Technology Review."
- Daniel Flowers of LLNL was quoted in the Wall Street Journal (September 28, 2004), discussing the potential benefits of HCCI engines.
- Daniel Flowers delivered an invited lecture at the SAE HCCI TopTech seminar, conducted in Berkeley, California, August 2004.
- John Dec was an invited speaker and panelist for an SAE panel discussion on HCCI at the 2003 SAE Fall Powertrain and Fluid Systems Conference, Pittsburgh, PA, October 2003.
- John Dec was an invited speaker at the SAE Homogeneous Charge Compression Ignition Symposium, Berkeley, CA, August 2004.
- John Dec was invited to present a keynote address on HCCI and advanced combustion at the 2004 SAE Fall Powertrain and Fluid Systems Conference, Tampa, FL, October 2004.
- The paper titled "Lattice-Boltzmann Diesel Particulate Filter Sub-Grid Modeling - a progress report", by George Muntean, D. Rector, D. Herling, D. Lessor and M. Khaleel of PNNL was selected for inclusion into SAE Transactions.
- A 2004 Advanced Combustion Engine R&D Special Recognition Award "For technical excellence and admirable collegiality in inter-laboratory collaborative research" was given to PNNL and ORNL for their work on emission controls for diesel-powered vehicles
- Peter Witze was given the SAE award for "Excellence in Oral Presentation" for his presentation at the SAE 2004 World Congress on high-energy, pulsed laser diagnostics for the measurement of diesel particulate matter.
- Stuart Daw, ORNL, and Dick Bint, GM were recipients of the annual DOE Advanced Combustion Engine Technical Achievement Award for their work in CLEERS.

- Robert Wagner received ORNL's Early Career Award for technical achievement and leadership in 2004.
- Dr. Johnney B. Green, Jr., was recognized as one of the "50 Most Important Blacks in Research Science" for 2004. The selection was based on his contributions to automotive research and his highly visible role as a minority scientist and role model to students and others. The "50 Most Important" are featured in the September edition of Science Spectrum magazine.
- John Storey, ORNL, was an invited speaker at the Advanced Collaborative Emissions Study (ACES) Workshop.

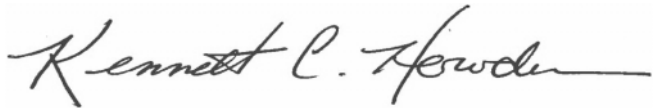
### **Invention and Patent Disclosures**

- U.S. Patent 6,736,106 awarded May 2004, "Engine Valve Actuation for Combustion Enhancement," R.D.Reitz, C.J. Rutland, R. Jhavar (University of Wisconsin).
- U.S. Patent 6,716,783 awarded April 6, 2004, "Catalysts for Lean Burn Engine Exhaust Abatement," K.C. Ott, N.C. Clark, M.T. Paffett. [LANL]
- "Novel Catalyst for Selective NO<sub>x</sub> Reduction Using Hydrocarbons," C. L. Marshall and M. K. Neylon (European patent application WO 03/031781 A1; April 17, 2003).
- "Novel Catalyst for Selective NO<sub>x</sub> Reduction Using Hydrocarbons," C. L. Marshall and M. K. Neylon (U.S. patent application 2003/0073566 A1; April 17, 2003).
- Patent application: "Catalyst and method for reduction of nitrogen oxides," Kevin C. Ott, DOCKET NUMBER: S-100,615. [LANL]
- "A New Concept and Catalysts for Lean-NO<sub>x</sub> Reduction", J.-H. Kwak, J. Szanyi and C.H.F. Peden of PNNL (invention disclosure filed December 12, 2003).
- "Sulfur removal via flash separation for on-board fuel utilization," patent pending, May 2004, for the work of Darrell Herling, et.al., of PNNL.
- "Method of generating hydrocarbon oxygenates from diesel, natural-gas and other logistical fuels," patent pending, May 2004, for the work of Darrell Herling, et.al., of PNNL.
- Accelrys filed a provisional patent on 12/01/2003 for inventions that were created while developing the CombiMat 2.5 database. The provisional patent, titled "Method of storing fast throughput experimentation information in a database," refers to four inventions.
- A patent has issued for the oxygen sensor (US 6,592,731) and for the Combined Oxygen and NO<sub>x</sub> Sensor (US 6,824,661).
- Portable LII Based Instrument and Method for Particulate Characterization in Combustion Exhaust; US patent No. 6,700,662 awarded to ANL.
- Patent awarded to Cummins Engine Company for an air/oil coalescer with improved centrifugally assisted drainage, Patent No. 6,640,792.
- Patent awarded to Cummins Engine Company for a valve train with a single camshaft, Patent No. 6,390,046.
- A patent has been allowed on a high-performance intake port invented by Charles Mendler. The port exhibits industry-leading flow values, which increases engine torque and reduces boost pressure requirements for engine down-sizing. The port was developed with funding from the U.S. Department of Energy. The publication number and date have not yet been issued.
- Patent application: "Boron carbide films and quantum well structure with improved thermoelectric properties," P. M. Martin and L. C. Olsen of PNNL.
- Patent application: "Integrated self-cleaning window assembly for optical transmission in combustion environments," Michael D. Kass and William P. Partridge Jr., DOE Invention DOCKET NUMBER: S-99,227 (ID1057). [ORNL]

The remainder of this report highlights progress achieved during FY 2004 under the Advanced Combustion Engine R&D Sub-Program. The following 59 abstracts of industry, university, and national laboratory projects provide an overview of the exciting work being conducted to tackle tough technical challenges associated with R&D of higher efficiency, advanced internal combustion engines for light-duty, medium-duty, and heavy-duty vehicles. We are encouraged by the technical progress realized under this dynamic Sub-Program in FY 2004, but we also remain cognizant of the significant technical hurdles that lie ahead, especially those to further improve efficiency while meeting the EPA Tier 2 emission standards and heavy-duty engine standards for the full useful life of the vehicles. In FY 2005, we look forward to working with our industrial and scientific partners to overcome additional barriers that hinder the wide-spread availability of high efficiency clean advanced internal combustion engines.



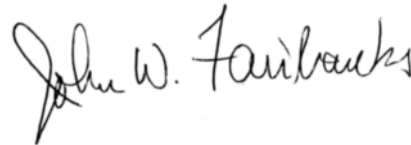
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